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13. ABSTRACT (Maximum 200 words)

Computational and asymptotic analyses were completed for the structures of wet carbon-monoxide flames. Both premixed flames and diffusion flames were considered. It was established that hydrogen-containing species affect burning velocities and extinction limits of these flames down to hydrogen concentrations of about one part per million. Reduced chemistry was derived for these flames in the vicinity of this limit as well as above and below it. In particular, useful one-step descriptions were obtained. The results can be applied to determining flammability limits and to predicting influences of water hydrogen addition to dry carbon-monoxide systems.

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Final Technical Report

The student supported by this grant, Maria Rightley, has successfully completed her Ph.D. and is now at Los Alamos National Laboratories. As indicated in the annual reports, she worked on reduced chemistry for premixed wet CO flames. Summaries of her publications and thesis are as follows:

The initial paper was published in *Combustion and Flame* 101:287-301 (1995). A summary of that work entitled "Analytical Approximations for Structures of Wet CO Flames with One-Step Reduced Chemistry" is as follows:

Since hydrogen-containing species catalyze CO oxidation, at small H/C and H/O ratios steady-state approximations for reaction intermediaries should be accurate and should produce a good one-step reduced-chemistry approximation for describing the flame structure. Such an approximation is complicated, however, because of the many elementary kinetic steps involved. In this work simplifications were introduced into one-step approximation that enable analytical expressions to be obtained for the burning velocities of premixed laminar flames by asymptotic methods. The resulting burning velocities were shown to be in good agreement with experiment and with detailed numerical predictions, and qualitative aspects of the internal flame structure were shown to agree with those deduced from full-chemistry numerical calculations. Estimates were given of the ranges of conditions over which the approximations can reasonably be employed and of flammability limits controlled by chemical kinetics.

The second paper, entitled "Burning Velocities of CO Flames", has been accepted for publication in *Combustion and Flame*. A summary of that work follows:

Asymptotic and computational methods were employed to investigate premixed laminar burning velocities of planar adiabatic flames in ideal gas mixtures containing carbon monoxide, oxygen, an inert and trace amounts of hydrogen-containing species. The chemical-kinetic steps that control the burning velocity were identified, and the dependence of the burning velocity on composition, pressure and temperature was determined. A lower limit to the burning velocity that is greater than 5 mm/s, independent of pressure, was established for totally dry stoichiometric mixtures at 300 K. The results contribute to understanding of CO flame structure.

The third paper, entitled "Structures of CO Diffusion Flames Near Extinction", is under consideration for publication in *Combustion Science and Technology*. A summary of that work follows:

Computational results were reported for structures of laminar counterflow diffusion flames between carbon monoxide and air, initially at room temperature and pressure from 1 to 100 atm, with total hydrogen-atom mole fractions in the system ranging from zero to about 0.002. All strain rates considered were within a factor of ten of the critical extinction strain rate. This critical strain rate was calculated as a function of pressure and of hydrogen content and was shown to lie below measured values under most condition. For hydrogen-free flames, activation-energy asymptotics were employed and support the computational results. It was reasoned that trace hydrogen amounts in air and preferential hydrogen diffusion through nonplanar diffusive-thermal instability contribute to enhanced flame robustness in the experiments, while increasing buoyant connective heat loss with increasing pressure promotes extinction at the higher pressures.

The title of Maria's Ph.D. thesis at UCSD, successfully defended in 1996, is "Numerical Analysis of Carbon Monoxide Flames by Reduced Kinetic and Asymptotic Methods". A summary of its contents is as follows:

The objective of study for this thesis was to gain insight into the chemical kinetics and physics that contribute to the structure and other characteristics of laminar flames which consume carbon monoxide. These laminar flames consisted of premixed flames and non-premixed (diffusion) flames. The methods for analyzing these flames included full-chemistry numerical calculations, reduced-chemistry numerical and analytical calculations, and analytical asymptotic calculations. The fuel was dry and wet carbon monoxide (CO), the wet containing various small amounts of hydrogen-containing (wet) species.

The first project involved premixed wet CO flames. For comparison, calculations with a 21-step mechanism were initially done. Then simplifications were introduced into a one-step approximation to enable analytical expressions to be obtained for the burning velocities using asymptotic methods. Comparisons were made with experimental values, and the ranges of conditions over which the approximations could reasonable be employed were determined. Additionally, approximate flammability limits for this flame were also calculated and compared to experimentally obtained values.

Wet and dry CO diffusion flames were also studied. Full-chemistry calculations, as well as reduced-chemistry calculations for the dry conditions, were performed for comparison with experimental results at atmospheric and higher pressures. The strain rate at which extinction occurred was one variable of particular interest. The full-chemistry mechanism consisted of 67 reactions, and as above, simplifications of the steady-state expressions for the species were introduced for the dry conditions to facilitate the calculation of extinction phenomena, and the chemical kinetics of the wet conditions were also explored.

This research is relevant to both premixed and nonpremixed combustion processes in propulsion and advances our knowledge of the combustion mechanism of flames involving carbon monoxide. It provides fundamental information that can be useful in future applications.